

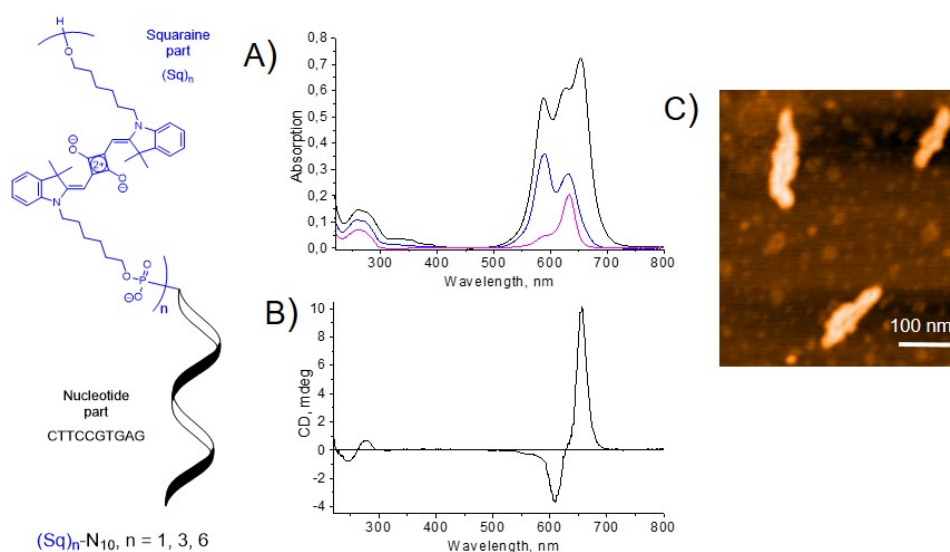
## Aggregation of a squaraine-modified oligonucleotide in aqueous solution

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Squaraine-based compounds are promising chromophores for the creation of new materials for biomedical or diagnostic applications through the methods of supramolecular chemistry. Squaraine dyes exhibit a molar absorptivity of up to 260 000 M<sup>-1</sup>cm<sup>-1</sup>. They absorb and emit light in the long-wavelength region of the visible spectrum. Furthermore, they tend to form well-ordered aggregates in organic and aqueous solutions.

In this work, we study the aggregation properties of oligomers which consist of squaraines (1, 3, or 6 molecules) and nucleotides (10 units). Their aggregation properties are studied by spectroscopic (UV-Vis and CD) and microscopic (AFM and TEM) methods in water/ethanol solutions (see Figure below).



A) UV-Vis spectra of the oligomers: **(Sq)<sub>1</sub>-N<sub>10</sub>** (magenta, no aggregation), **(Sq)<sub>3</sub>-N<sub>10</sub>** (blue, H-aggregation), and **(Sq)<sub>6</sub>-N<sub>10</sub>** (black, oblique aggregation) B) CD spectrum and C) AFM image of the **(Sq)<sub>6</sub>-N<sub>10</sub>** oblique aggregates

Based on UV/vis spectroscopy, oligomer **(Sq)<sub>1</sub>-N<sub>10</sub>** with one squaraine molecule shows no well-defined type of aggregation. Oligomer **(Sq)<sub>3</sub>-N<sub>10</sub>** containing three squaraine units, however, reveals stacking of the chromophores in H-type fashion (blue shifted absorption band). Finally, oligomer **(Sq)<sub>6</sub>-N<sub>10</sub>** can form both H-type and oblique (splitting of the absorption band) aggregates depending on the conditions of preparation. The oblique aggregates of the **(Sq)<sub>6</sub>-N<sub>10</sub>** exhibit the signs of the supramolecular polymers, in which the squaraine-nucleotide oligomers are arranged in a helical fashion.